Estra-1,3,5(10)-trien-17-one, 3-(acetyloxy)-

Other names:	Estrone, acetate
	Estrone 3-acetate
	Hogival
	Oestrone-3-acetate
	3-Acetoxyestrone
	3-Acetoxyestrone R
	3-Hydroxyestra-1,3,5(10)-17-one acetate
	3Beta-acetoxyestra-1,3,5(10)-trien-17-one
	3-(Acetyloxy)-estra-1,3,5(10)-trien-17-one
Inchi:	InChI=1S/C20H24O3/c1-12(21)23-14-4-6-15-13(11-14)3-5-17-16(15)9-10-20(2)18(17)7-8
InchiKey:	KDPQTPZDVJHMET-PNYFIKQUSA-N
Formula:	C20H24O3
SMILES:	CC(=O)Oc1ccc2c(c1)CCC1C2CCC2(C)C(=O)CCC12
Mol. weight [g/mol]:	312.40
CAS:	901-93-9

Physical Properties

Property code	Value	Unit	Source
gf	-0.99	kJ/mol	Joback Method
hf	-424.06	kJ/mol	Joback Method
hfus	28.09	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.037		Crippen Method
mcvol	245.330	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	2397.00		NIST Webbook
rinpol	2397.00		NIST Webbook
tb	862.08	K	Joback Method
tc	1111.39	K	Joback Method
tf	573.44	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.63	J/mol×K	862.08	Joback Method
cpg	842.84	J/mol×K	903.63	Joback Method
cpg	863.41	J/mol×K	945.18	Joback Method
cpg	883.57	J/mol×K	986.73	Joback Method
cpg	903.54	J/mol×K	1028.29	Joback Method
cpg	923.55	J/mol×K	1069.84	Joback Method
cpg	943.84	J/mol×K	1111.39	Joback Method
hfust	15.00	kJ/mol	399.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C901939&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume